

FUTURE MM/SUBMM INSTRUMENTATION AND SCIENCE OPPORTUNITIES: EXAMPLE OF DEUTERATED MOLECULES

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ABSTRACT

During the next decade a tremendous advance will take place in instrumentation for spectroscopy of the interstellar medium. Major new facilities (ALMA, SOFIA, APEX, LMT, Herschel and others) will be constructed and commissioned, so that the science opportunities, in the field of astrochemistry, will increase by a huge factor. This will be enhanced by the new receivers with greater bandwidth and sensitivity. The new opportunities will be in the area of astrochemistry of distant objects, through greater sensitivity, or new spectral ranges due to the platforms above the Earth's atmosphere.

Various aspects of new spectral ranges are discussed, with emphasis on H₂O lines, features previously hidden under H₂O or O₂ lines, light hydrides and particularly on deuterium in molecules. Recently, multiply deuterated species have been detected, e.g. ND₃, in cold dense regions of the interstellar medium. It is argued here that it is possible that so much deuterium could be trapped, by the fractionation process, into heavy molecules such as ND₃, etc..., and species such as H₂D⁺ and possibly D₂H⁺, that D and HD might be depleted. This would be the mechanism for the large dispersion of [D]/[H] values found in the interstellar medium. Light molecules (hydrides and deuterides) generally have large fundamental rotation frequencies, often lying in the HIFI bands. The deuterides are a specially suitable case, because the species exist mainly in cold dense regions, where the molecules are in the ground states and THz observations will best be carried out by absorption spectroscopy against background dust continuum sources such as Sgr B2 and W49N.

Key words: ISM: molecules – Astrochemistry – Deuterium – Submillimeter

1. INTRODUCTION

A great deal is already known about the nature of the gas and dust in the interstellar medium, obtained from a wide variety of telescopes and facilities. Most of these have been ground-based, but some airborne, balloon-borne, or space missions. In particular, high resolution, heterodyne ($R \geq 10^6$) spectrometers have provided information on the molecular and (surprisingly) atomic species in the various types of interstellar clouds. It has indicated the physical nature of the gas, mostly from the velocity structure and tested the chemical models, e.g., the ion-molecule reaction scheme, which was of course developed to explain the observed molecular content of the clouds. Figure 1 (Phillips & Keene 1992) shows a submillimeter and far-infrared spectrum of an interstellar cloud, as it might be observed from a space platform. Features include the line-forest of heavy molecules at the longer wavelengths, light hydrides and deuterides at shorter wavelengths, important atoms and ions, such as C⁰, C⁺, O⁰... and dust continuum and resonances. Also large molecules are possibly to be seen via their bending modes.

Compared to other branches of astronomy, the submillimeter has been slow to develop, in part due to the low photon energy (compared to optical) and the small number of arriving photons (compared to the radio), making it difficult to construct detection equipment, but also due to the poor overall transmission of the Earth's atmosphere. As is seen in Figure 2 (top), even from a high mountain site such as Mauna Kea, Hawaii, the transmission is only partial up to about 900 GHz (330 μ m) and very little above that. Of course, from airborne altitudes, i.e., 12 km for SOFIA, transmission is much better (Figure 2, bottom) but is still badly interrupted by H₂O and O₂ lines. There is a clearly indicated need for space-based telescopes.

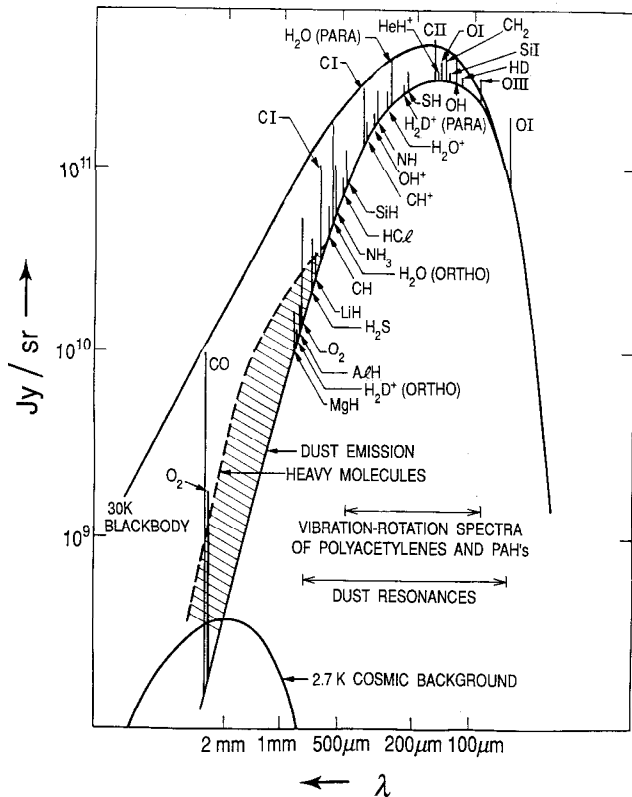


Figure 1. Illustration of the principal spectral lines expected at submillimeter wavelengths, shown superposed on the dust continuum emission of a 30 K interstellar cloud.

A third, and possibly dominant reason for the underdeveloped nature of the field is the lack of major instruments. Because the millimeter/submillimeter observers are developing their field later, in time, compared to the optical, radio and X-ray communities, we have had to wait our turn for major funding. The wait is almost over and the full potential of this exciting field is about to be realized in the coming decade!

2. NEW INSTRUMENTS

We are concerned with the new opportunities for interstellar chemistry, which include investigation of molecules and atoms in the gas phase, dust grains and surface chemistry and the interactions between the gas and dust phases, including accretion of molecules onto grains, and the opposite process, where the accretion material is returned to the gas phase. Here, we discuss this only from the point

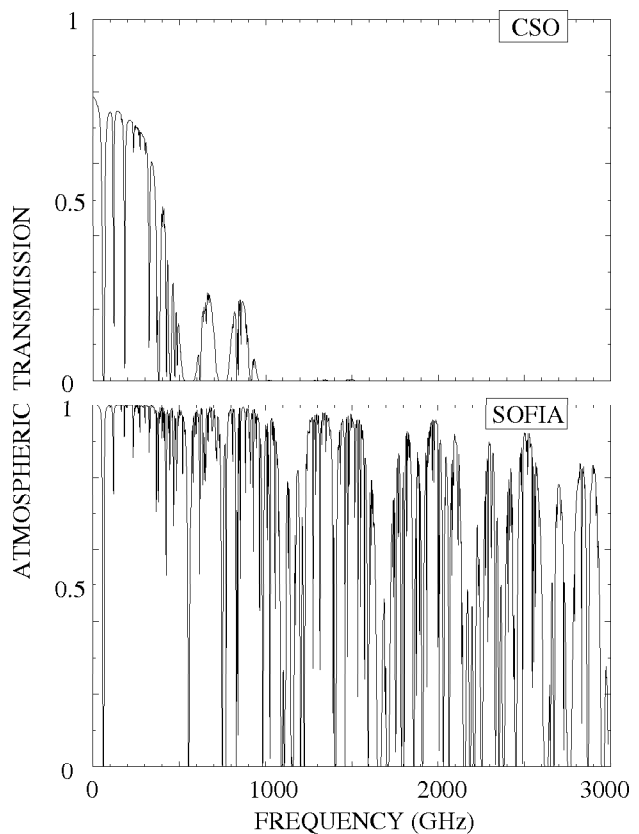


Figure 2. Comparison of the atmospheric transmissions between the sky visible at CSO (with a standard precipitable water column of 1 mm) and the sky that will be visible for SOFIA (with a standard precipitable water column of 10 μ m), both at an elevation of 45°.

of view of gas spectroscopy.

Table 1 lists many of the major new telescopes and interferometers which will be available within the next decade (hopefully).

Compared to what we have today, this will be a staggering new capability and the field will lead astronomy in that it will discover and define the new objects and new concepts to be investigated. One might worry that there will not be enough trained people in the field to fully utilize such a cornucopia of facilities, so university-based facilities should expand their efforts in this field now! ALMA represents the biggest step forward, providing an unprecedented spectroscopic capability, throughout the atmospheric windows, for nearby and distant objects. This huge sensitivity will probably manifest itself most dramatically for nearby objects in the chemistry of prestellar

Table 1. New facilities for interstellar chemistry.

Name	Aperture	Platform	Available
SOFIA	2.5 m	Airborne (747)	2005
Herschel	3.5 m	Space (L2)	2007
ALMA	64 × 12 m	Atacama (Chile)	2010
CARMA	6 × 10 m	White Mts (California, USA)	2005
SMA	8 × 6 m	Mauna Kea (Hawaii, USA)	2003
e-SMA	(8 × 6 m) + 15 m + 10 m	Mauna Kea (Hawaii, USA)	2005
LMT	50 m	Sierra Negra (Mexico)	2004
APEX	12 m	Atacama (Chile)	2005
South Pole	8 m	South Pole	2006
GBT	100 m	West Virginia (USA)	2002

disks around Young Stellar Objects (YSOs), and at the other end of the distance scale, for the chemistry of the interstellar medium of primordial galaxies. One caveat might be mentioned: high spectral resolution is often required where there is high spatial resolution. Even with single-dish beams of $30''$, local galaxies such as Cen A show disk features of only 10 km s^{-1} in width. Thus, ALMA must provide correlator capability for high spectral resolution ($\sim 1 \text{ km s}^{-1}$) at full galaxy bandwidths ($\geq 1000 \text{ km s}^{-1}$) on as many baselines as possible.

ALMA will make images, at 1 mm wavelength, with the same ($0.1''$), or better resolution than achieved by the Hubble Space Telescope (HST), at visible wavelengths. This capability will enable many new imaging programs, including:

1. Studies of the evolution of dust and gas from molecular clouds, to circumstellar disks, to planetary systems;
2. Studies of the enigmatic hot cores across the Galaxy;
3. Studies of YSOs across the Galaxy;
4. Investigations of the chemistry of circumstellar disks, using multiple lines of many species, possibly by means of line-surveys;
5. Measurements of cloud temperatures across the Galaxy, for studies of depletion in cold cores and chemical fractionation.

SOFIA, the new NASA airborne observatory, will give an improved view of much of the region of the spectrum blocked by the atmosphere. With a 2.5 m telescope and much improved spectrometers compared to the KAO, many specific new spectroscopic features can be searched for, with the exception of H_2O and O_2 lines, and features

still hidden by the strong atmospheric lines. Ultimately the spectroscopy of the interstellar medium and nearby galaxies will be best studied from HIFI, the heterodyne instrument on Herschel, the ESA cornerstone mission. At the L2 point, an ideal satellite location, studies such as line-surveys can be carried out continuously in time and without interruption from H_2O atmospheric lines. Both SOFIA and Herschel will extend the high quality spectroscopy range to about 2 THz or possibly more.

Actually, in spite of the impressive size and cost of the new instruments, much of the new capability is provided by the smallest component: the detector element. Since their inception (~ 1979), SIS devices have increased sensitivity by a factor approaching 100. Now, essentially quantum noise limited, the route to further improvement is in more bandwidth and more sophisticated device structure. For instance, IF bandwidths are at about 4 GHz and are planned for as much as 20 GHz. For single-dish work, the single junction element is being replaced by devices detecting both polarizations, having instantaneous on-off subtraction, sideband separation, and possibly balanced mixing. Each of these features implies the use of two junctions, thus up to 16 detectors could be used for spectroscopy of a distant point source, resulting in a sensitivity gain of about 5 or so. Similarly, the increased frequency range ($\sim 2 \text{ THz}$) is being supported by new beam-lead, broad band, high output power, diode multipliers for the local oscillators.

3. NEW SPECTRAL OPPORTUNITIES

While ALMA provides sensitivity and angular resolution breakthroughs, SOFIA and Herschel (HIFI) generate the opportunity for observing in new spectral ranges, due to the avoidance of some or all of the atmospheric H_2O . HIFI will provide a novel view of much of the submillimeter spectrum, totally unperturbed by atmospheric H_2O . It was intended that HIFI would have total frequency coverage from about 480 GHz to 2.7 THz, but the technical difficulty of production of the local oscillators, combined with the limited budget and fixed launch schedule, has forced the abandonment of the highest frequency channel, so the highest frequency now is 1.9 THz (the frequency of the C^+ line).

3.1. LINE-SURVEYS

Much of the HIFI data will be taken in the form of line-surveys. These have been spectacularly successful on ground-based telescopes (see Figure 3), and the methodology has been refined by means of simulations (Comito & Schilke 2001), to make it suitable for rapid frequency scanning, such that a full spectral survey of THz bandwidth can be completed, by HIFI, for strong sources in a day or less. This compares with the many weeks taken on ground-based telescopes to obtain only 100 GHz of data. The factor ~ 100 of improvement in time is mostly due to the automation necessary for space and the vastly improved designs of mixers and local oscillators.

3.2. H_2O

Some H_2O lines have been observed from the ground and from the KAO, but the bulk of observations is of the 557 GHz line from SWAS and also ODIN. Figures 4 and 5 show some amazing SWAS H_2O spectra, indicating a complex structure to the line shape, often including self absorption. The three sources presented in these figures are Sgr B2 (Neufeld et al. 2000), W51 (Neufeld et al. 2002) and W49N (Plume et al. *in preparation*). These are distant compact HII regions, where absorption lines observations can trace the water vapor content in clouds along their line of sight.

HIFI will have available many transitions of H_2O and H_2^{18}O , most of which have not been observed previously, including those in the important excitation path to the ground-state (Figure 6).

These many available transitions will probe the gas cooling properties of H_2O in objects with a wide range of densities, such as collapsing protostellar envelopes (Cec-

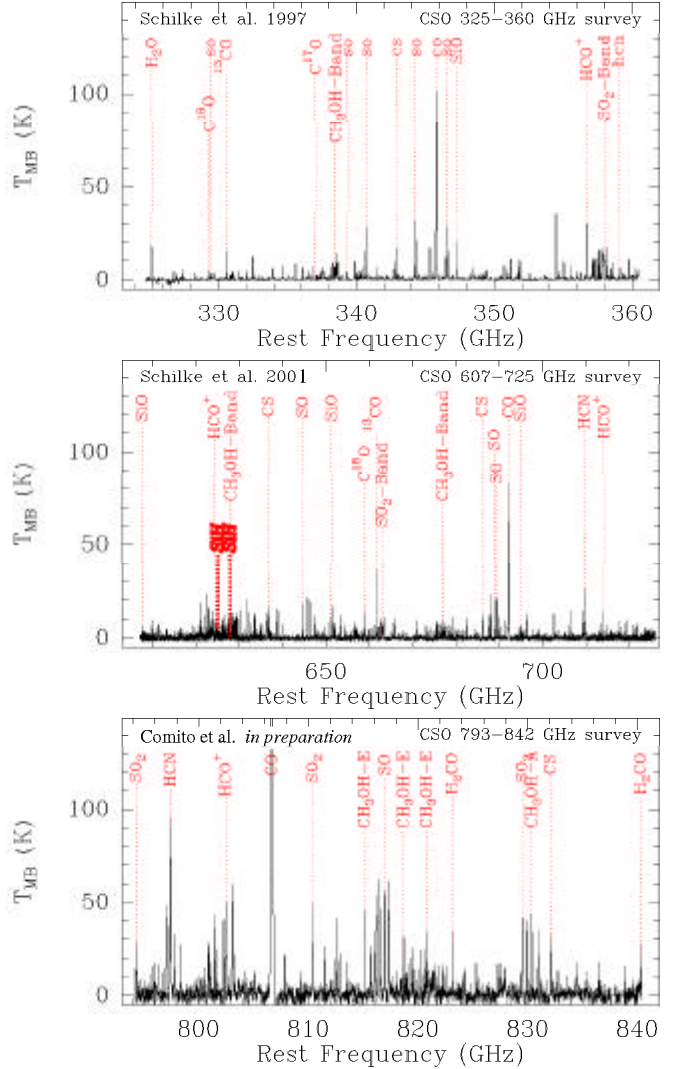


Figure 3. Line-surveys of Orion with the CSO telescope.

carelli et al. 1996), where H_2O becomes the primary coolant as the density increases in the inner regions.

3.3. HIDDEN SPECIES

Besides the H_2O lines themselves, there exists a body of spectral features never observed because of their proximity in frequency to the H_2O and O_2 lines. Some examples are lines of H_2D^+ (e.g. $2_{1,1} \rightarrow 2_{1,2}$ at 1.112 THz), CH^+ (e.g. $1 \rightarrow 0$ at 836 GHz), NH (e.g. $N = 1 \rightarrow 0$, $J = 0 \rightarrow 1$ at 946 GHz) and LiH (e.g. $1 \rightarrow 0$ at 444 GHz). Molecular lines such as HCl ($1 \rightarrow 0$) at 626 GHz and SiH at 627 GHz are hard to observe from the ground, being in the wings of H_2O lines. Many of the “hard to detect from the

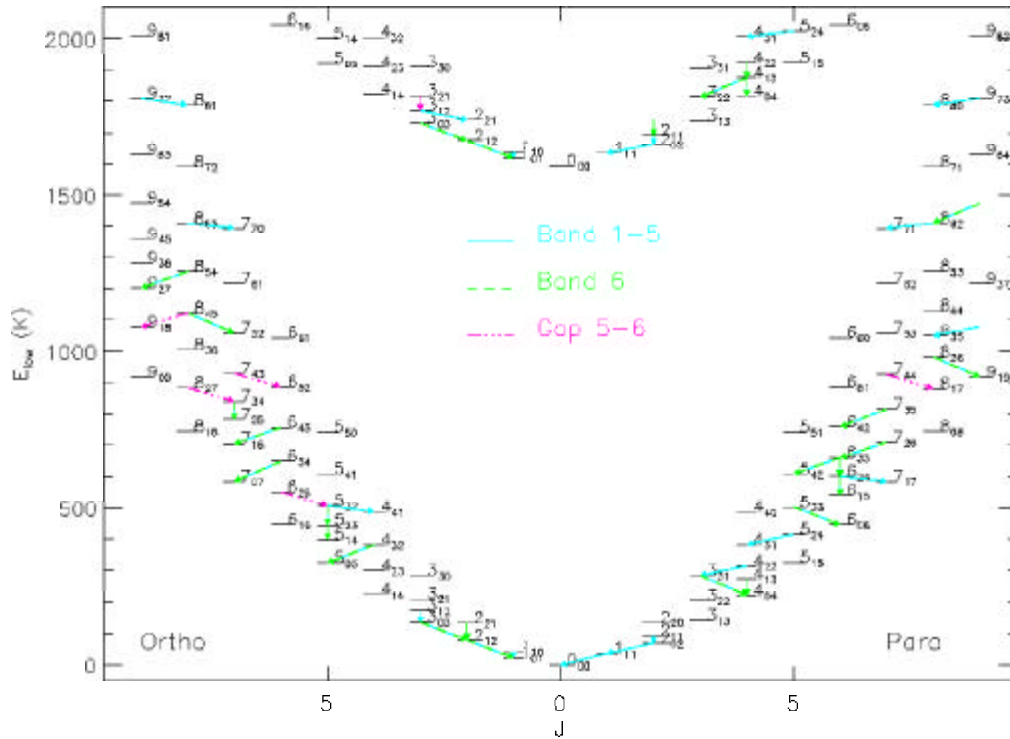


Figure 6. Water transitions available to HIFI. Bands 1-5 covers the frequency range 472-1280 Gz; Band 6 covers 1400-1904 GHz; Gap 5-6 is the frequency range between Band 5 and Band 6, which may not be covered.

ground” species are light, fast rotators, typified by the diatomic hydrides. Some of these, e.g. NaH, CaH, MgH,... have been searched for in $J = 0 \rightarrow 1$ transitions using atmospheric windows for ground-based telescopes, with negative results, but can be searched for now, with increased sensitivity, in two ways. The first method (can be carried out from the ground in favorable cases) makes use of cold clouds on the line of sight to powerful continuum sources, such as Sgr B2. There, in the cold dark clouds, the molecules will be in the ground state and would be detected in absorption. This method avoids the confusion in the spectra of GMCs, since the line forest is largely made up of highly excited molecular lines, which, of course, is not the case for the hydrides in cold clouds. A good example is seen in the SWAS detection of the ground-state H_2O line in Sgr B2 (Figure 4). The second method does suffer from GMC line confusion, but makes use of the new high frequency capabilities for HIFI and SOFIA, where the high J lines of the various hydrides will have much higher line strengths than $1 \rightarrow 0$; hopefully this will overcome the line-forest effect in the high temperature and

high density sources.

Generally, above 1 THz the almost zero atmospheric transmission has prevented studies so far, but several windows of limited size and strength have been recently detected on high sites. Space platforms will allow studies of HD ($1 \rightarrow 0$) at 2.67 THz, HeH⁺ ($1 \rightarrow 0$) at 2.01 THz, N⁺ at 1.46 and 2.46 THz, HF at 1.23 THz, FeH at 1.41 THz, OH at 1.83 THz, OH⁺ at 2.46 THz, etc... Some species have been detected by ISO, e.g. CH⁺ in the high J transitions (Cernicharo et al. 1997), HF (Neufeld et al. 1997) and HD (Wright et al. 1999, Caux et al. 2002). HIFI will be a great improvement compared to what used to be available on ISO.

4. DEUTERIUM

One of the most important aspects of molecular spectroscopy of the interstellar medium is the study of the abundance of deuterium. The new facilities will provide a much wider range of frequencies and sensitivities, so that the deuterium studies can be extended to new species and new objects. The fundamental aspect of deuterium

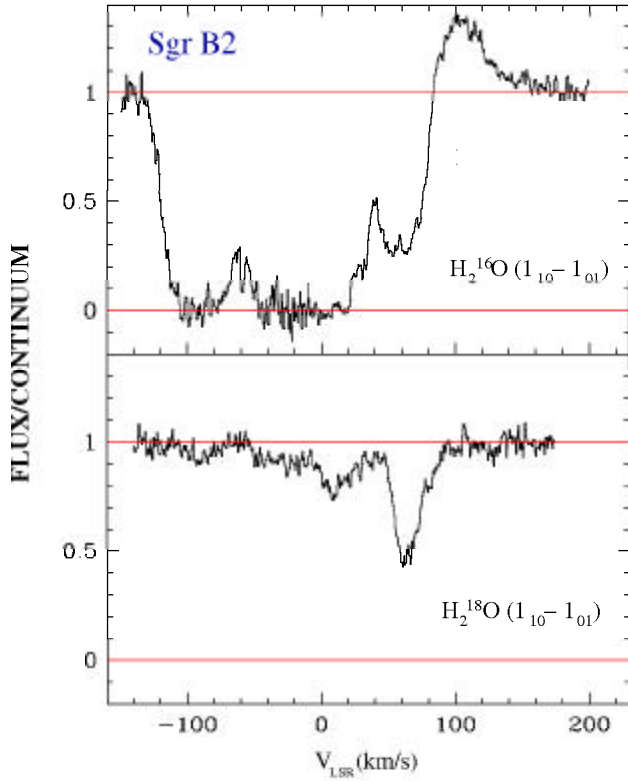


Figure 4. $H_2^{16}O$ and $H_2^{18}O$ line detections by the SWAS satellite toward Sagittarius B2.

chemistry is that the chemical fractionation process (see below) forces deuterium atoms into heavy molecules, at the expense of hydrogen, whenever the medium is cold, with amazing results.

Deuterium-bearing molecules have become the target of many observations in recent years and several models have been developed to account for them (Tielens 1983, Roberts & Millar 2000a, Roberts & Millar 2000b). More than twenty such molecules have been detected to date in interstellar clouds with abundances, relative to the non-deuterated counterpart, ranging from 10^{-1} to 10^{-4} . It is accepted that deuterium is produced during the Big Bang and it is generally believed that since the Big Bang, deuterium has been destroyed but not created in nuclear reactions occurring inside stars.

The most reliable determinations of the D/H ratio are based on spectroscopic measurements of Lyman series ultraviolet absorption lines from foreground interstellar gas. In our Galaxy, this has been obtained (via DI and

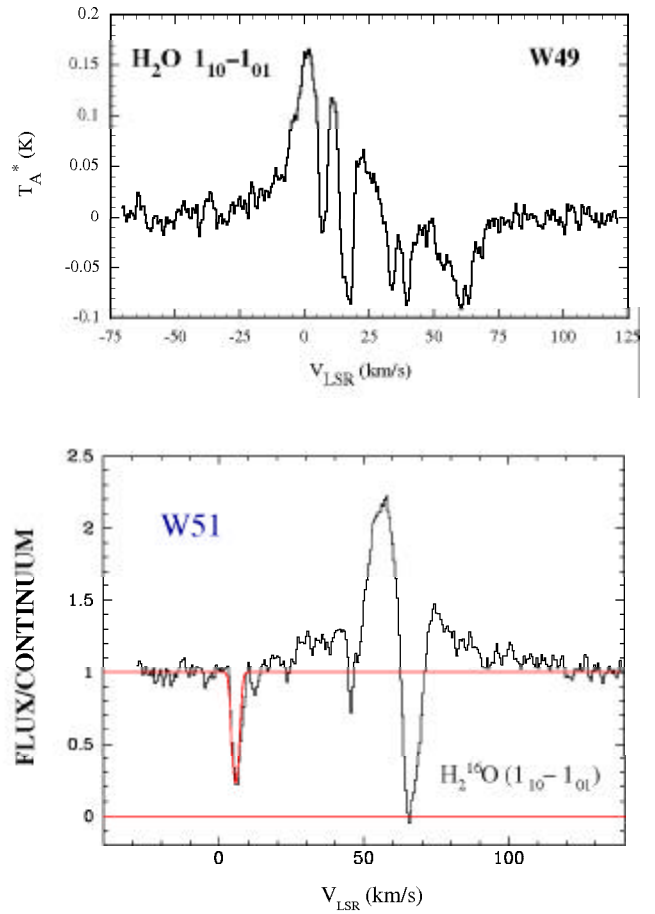


Figure 5. Two spectacular examples with W49N, a distant (~ 11.4 kpc) compact HII region whose line of sight crosses twice the Sagittarius spiral arm, and W51 located at ~ 7 kpc.

HI observations) with satellites such as the International Ultraviolet Explorer (IUE), Copernicus, the Extreme Ultraviolet Explorer (EUVE), the Hubble Space Telescope (HST) and recently the Far Ultraviolet Spectroscopic Explorer (FUSE). Measurements of the D/H ratio toward high-redshift systems like quasars (e.g. Tytler et al. 1999) seemed to show more dispersion than expected and an inverse correlation of this abundance with HI column density. If this is real, it would suggest that in these high HI column density systems, some processing of D/H must have occurred (Vidal-Madjar 2000, Fields et al. 2001). It is interesting to note that abundances of deuterium measured in the interstellar medium also appear to show considerable dispersion. From published values, D/H ranges from $\sim 5 \times 10^{-6}$ to $\sim 4 \times 10^{-5}$. FUSE observations of seven white dwarfs and sub-dwarfs lead to a D/H ra-

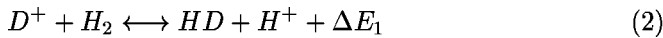
tio of $(1.52 \pm 0.08) \times 10^{-5}$ (Moos et al. 2002), to be compared with the value of $(1.5 \pm 0.1) \times 10^{-5}$ (Linsky 1998) determined from HST observations of late-type stars. Both measurements refer to warm interstellar gas, located within 100 pc of the Sun. However, differences by a factor of two have been derived from Copernicus and HST data toward stars located between 100 and 500 pc from the Sun. The ratio seems constant within 100 pc, but seems to vary at considerably greater distances. There is no identified process which can explain such large variability and without an understanding it is not justified to use an average D/H ratio to represent the primordial deuterium abundance. We will argue, below, that the chemistry of the interstellar medium could be responsible, in that it can extract large amounts of deuterium which becomes trapped in molecules and on grains.

4.1. BASIC CHEMISTRY

Deuterium bearing species are good probes of the cold phases of molecular clouds prior to star formation and many recent observations point to the fact that their abundance relative to their hydrogenated analogues are larger, by a factor up to 10000, than the solar neighborhood value of $\sim 1.5 \times 10^{-5}$ (see references above). Therefore the relative abundance of isotopomers does not measure the relative abundances of the isotopes themselves. The chemical fractionation process arises from differences in the molecular binding energies caused by the different zero-point vibration energy. Almost incredibly, this can lead to a detectable quantity of the triply deuterated ammonia (see section 4.2).

In molecular clouds, hydrogen and deuterium are predominantly in the form of H_2 and HD respectively. So the HD/ H_2 ratio should closely equal the D/H ratio. Since the zero-point energies of HD and H_2 differ greatly (see Figure 7), the chemical fractionation will favor the production of HD compared to H_2 .

Deuterium is initially removed from the atomic phase through charge exchange with H^+ , followed by reaction with the abundant H_2 . HD could further interact with D^+ again to give D_2 :



The reactions 2 and 3 are exothermic as substituting an H atom versus an D atom in a polyatomic molecule

generally leads to a gain in energy. These energies may be computed (at 0 K) by the differences between the zero-point energies of the products and the reactants. The energies ΔE_1 and ΔE_2 are quoted in figure 7.

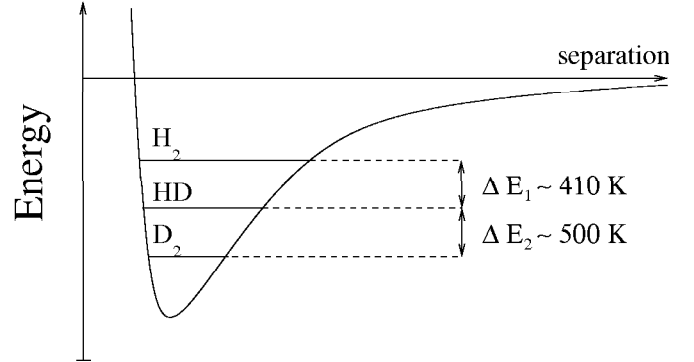
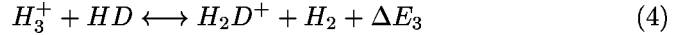


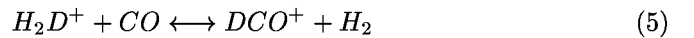
Figure 7. H_2 , HD and D_2 potential energy diagram. ΔE_i is the difference between the zero point energies relative to the minimum of the molecular potential curve.

In the dense, cold regions of the interstellar medium, D will be initially nearly all absorbed into HD. The abundant ion available for interaction is H_3^+ , which gives H_2D^+ :

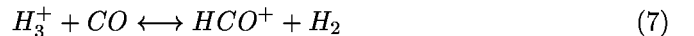


where $\Delta E_3/k \sim 230$ K for a typical temperature of a dark cloud of about 10 K (e.g. Millar et al. 1989). The reverse reaction does not occur efficiently in the cold dense clouds where obviously the temperature is much lower than ΔE_3 . Therefore, the degree of fractionation of H_2D^+ becomes non-negligible.

This primary fractionation can then give rise to a second fractionation:



In dark clouds H_3^+ gives rise to HCO^+ via the reaction:



4.2. MULTIPLY DEUTERATED MOLECULES

The study of doubly deuterated interstellar molecules has been booming in the last few years since the surprising discovery of a large amount ($\sim 5\%$) of doubly deuterated formaldehyde in the low mass protostar IRAS 16293-2422 (Ceccarelli et al. 1998, Loinard et al. 2000). This is more than one order of magnitude higher than in Orion KL where D_2CO was first detected by Turner (1990). This first discovery was followed by many other studies which

confirmed the presence of very large amount of doubly deuterated formaldehyde (D_2CO) as well as ammonia (ND_2H) (e.g. Roueff et al. 2000, Loinard et al. 2001). Gas phase chemical models account relatively well for the observations of the abundances of singly deuterated molecules but may not be able to completely reproduce the large deuterations observed for multiply deuterated molecules. The large deuterations could also be a product of active chemistry on the grain surfaces as predicted by Tielens 1983 with two processes:

1. Deuteration during the mantle formation phase;
2. Evaporation of the mantles ices resulting from the heating of the newly formed star, with injection into the gas phase of the deuterated species.

The year 2002 appears to be the cornerstone in the study of deuteration processes with the first detection of a triply deuterated molecule, ND_3 . Until now, the possibility for detecting triply deuterated molecules was so remote that their lines were omitted in the spectroscopic catalogs for astrophysics. The ground-state rotational transition at 309.91 GHz of ND_3 has been detected with the CSO towards the Barnard 1 cloud (Lis et al. 2002, see Figure 8) and the NGC 1333 IRAS 4A region (Van der Tak et al. 2002), with abundance ratios $[ND_3]/[NH_3] \sim 10^{-3}$ and $[ND_3]/H_2 \sim 10^{-11}$. They conclude that reactions in the gas-phase are more likely to produce these high degrees of deuteration, rather than grain surface chemistry. However they cannot totally rule out the possibility that surface processes also contribute to the formation of ND_3 (cf Rodgers & Charnley 2001). Recent observations of the extended D_2CO emission towards L1689N (Ceccarelli et al. 2002) pointed out the difficulty in explaining the D_2CO abundance, either with gas phase models or with grain surface chemistry. The many routes to deuteration are not fully understood and more observations are necessary to elucidate these processes. Very recently, doubly deuterated hydrogen sulfide has been detected by Vastel et al. (*in preparation*) with the CSO towards the Barnard 1 cloud and the DCO^+ ($3 \rightarrow 2$) emission peak of NGC 1333 IRAS 4A (see Lis et al. *in preparation*). Figure 9 shows as an example the first detection of D_2S ($1_{1,1} \rightarrow 0_{0,0}$) together with HDS ($1_{0,1} \rightarrow 0_{0,0}$).

4.3. DEPLETION OF CO

Gas phase species are expected to be depleted at the centers of cold, dark clouds, since they tend to stick to the dust grains. A series of recent observations has shown that, in some cases, the abundance of molecules like CO decreases toward the core center of cold, dense clouds

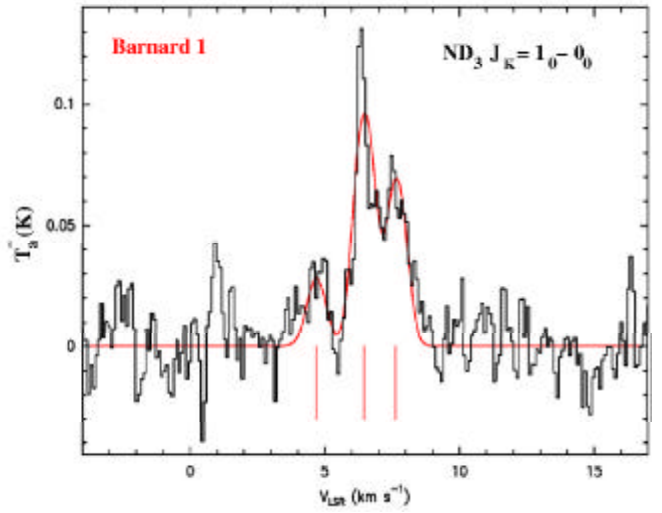


Figure 8. Spectrum of the 309.91 GHz ND_3 line towards Barnard 1 observed at the CSO. The red lines show the fits to the position and strength of the hyperfine components.

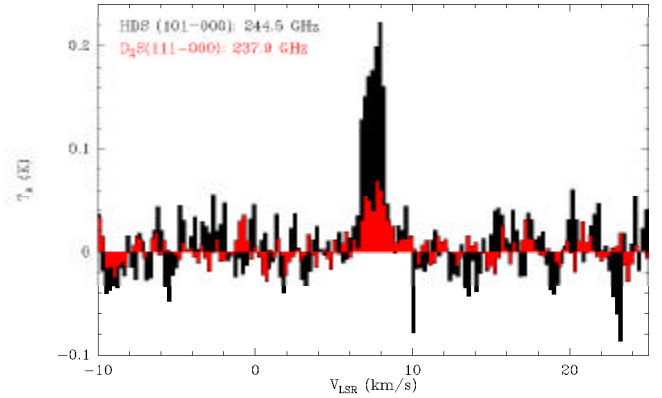


Figure 9. HDS ($1_{0,1} \rightarrow 0_{0,0}$) and D_2S ($1_{1,1} \rightarrow 0_{0,0}$) detections with the CSO towards the DCO^+ ($3 \rightarrow 2$) emission peak of NGC 1333 IRAS 4A (Vastel et al., *in preparation*).

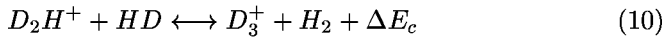
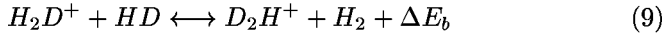
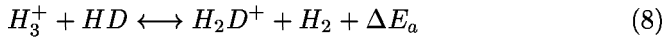
(L1498: Willacy et al. 1998; IC 5146: Kramer et al. 1999, Bergin et al. 2001; L977: Alves et al. 1999; L1544: Caselli et al. 1999; L1689B: Jessop & Ward-Thompson 2001; Bachmann et al. 2002). These decreases in abundance have been interpreted as resulting from the depletion of molecules onto dust grains (see, e.g., Bergin & Langer 1997; Charnley 1997). It is now clear that these drops in abundance are typical of all dense cores. The removal of these reactive species affects the gas-phase chemistry and particularly the deuterium fractionation within the cloud.

Indeed, the removal of species which would normally destroy H_3^+ (e.g. CO; Roberts & Millar 2000a) means that the H_3^+ is more likely to react with HD and produce H_2D^+ (reaction 4).

H_2D^+ has been detected toward the low luminosity proto-stars NGC 1333 IRAS 4A (Stark et al. 1999) and IRAS 16293-2422 (Stark et al. *in preparation*) with a H_2D^+/H_2 ratio of 3×10^{-12} in the former. Recently, Caselli et al. (*in preparation*) detected the H_2D^+ 372 GHz line towards two pre-stellar cores, L1544 and L1521F, both probably on the verge of collapse.

4.4. MODIFICATION OF THE DEUTERIUM CHEMISTRY

The large differences found in the values of the deuterium abundance in the interstellar medium pose the question as to the mechanisms responsible for these variations. A possible answer is the chemical fractionation process, which, in cold regions of the interstellar medium, steadily forces the deuterium into the heavy molecules. The trend, is to minimize the free energy, which implies forming the heaviest species, with the least uncertainty energy (see Figure 10). As shown in the previous section, in the very cold (~ 10 K) regions where, e.g. ND_3 is detected, CO is in fact heavily depleted by accretion on to grains. For example, $[CO/H_2] \sim 5 \times 10^{-6}$ (Bacmann et al. 2002), leaving HD at $[HD/H_2] \sim 5 \times 10^{-5}$ as the most abundant molecule available for reaction with H_3^+ and H_2D^+ . Another example is the case of HD 112 μm absorption towards a cold molecular cloud in the line of sight of W49 where Caux et al. (2002) found that HD is 12 times more abundant than CO. The result may be the production of more high deuterium content molecules:



where ΔE_a , ΔE_b and ΔE_c are the released energies of the exothermic reactions. Using the zero-point energies computed by Carney (1980), and the energy of the first allowed rotational state of the H_3^+ molecule permitted by the Pauli exclusion principle (~ 92 K), these values are: $\Delta E_a \sim 230$ K, $\Delta E_b \sim 180$ K and $\Delta E_c \sim 230$ K.

The species D_2H^+ may indeed be detectable in sufficiently cold, CO depleted regions. Because of the low temperature of the highly deuterated regions (~ 10 K), the lowest lying transition of H_2D^+ and D_2H^+ will be most appropriate and can be searched for in absorption against Sagittarius B2, possibly:

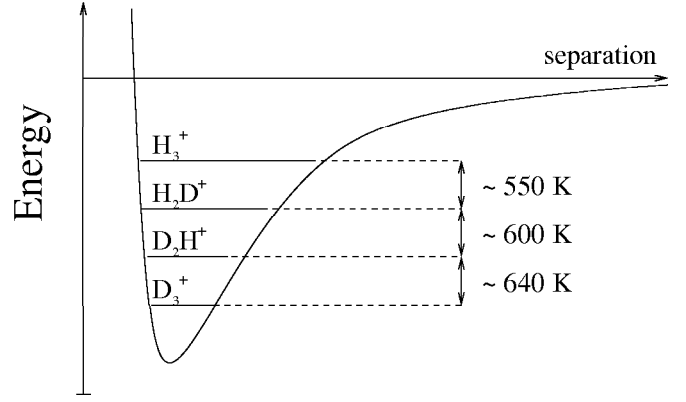


Figure 10. H_3^+ , H_2D^+ , D_2H^+ and D_3^+ potential energy diagram.

- $H_2D^+_{101-000}$ at 1370.15 GHz *
- $H_2D^+_{211-212}$ at 1111.74 GHz
- $D_2H^+_{111-000}$ at 1476.60 GHz
- $D_2H^+_{220-211}$ at 1370.05 GHz *

* It appears to be purely chance that these frequencies are so close.

4.5. D, HD DEPLETED BY FRACTIONATION?

It would be a difficult task to make an inventory of all D substituted molecular species throughout the Galaxy, to see if the measured values of the deuterium abundance could be affected. The fractionation might work in favor of metal species (e.g. ND_3) in high metallicity galaxies, or in favor of purely hydrogenic species (e.g. H_2D^+ and D_2H^+) in low metallicity objects. At any rate, we can ask if it is physically possible for the former case to occur. If we take the local value of C, N and O abundances and count the total number of bonds available for substitution of H by D, we get 3×10^{-3} [H]. But $[D]/[H]$ is only $\sim 10^{-5}$, so there does exist the possibility of such an effect. In fact, if the product of the fraction of available bonds actually occupied by D (f_D) times the fraction of the interstellar medium which is cold enough for strong fractionation and CO depletion (f_C) approaches 10^{-3} , then there will be a significant effect:

$$f_D \times f_C \geq 10^{-3} \quad (11)$$

We know that $f_D \sim 10^{-1}$, or more in some cases, so if $f_C \geq 10^{-2}$, measured values of the deuterium abundance may be significantly affected.

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